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APPLICATION OF A THREE-DIMENSIONAL PHOTOCHEMICAL SMOG FORMATION MODEL TO THE TOKYO METROPOLITAN AREA

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16. ABSTRACT

Relatively high O_3 concentrations were observed during an episode on July 16 and 17, 1981 in the Tokyo Metropolitan Area. The stagnant meteorological conditions which existed then were mainly caused by the local sea and land wind circulation systems. To better understand the physical and chemical relationships at work during this particular episode the SAI Urban Airshed Model (UAM) was applied. Vertical cross-sections of simulated pollutant patterns are analyzed for the Tokyo domain, including the diurnal variation in the patterns. The effects of vertical meteorological conditions and the previous day's secondary pollutants are emphasized. The entrainment of O_3 and CARB from aloft on the second day of simulation was shown to have significant impact on the timing and location of the second day's maximum O_3. Limited field-observed data from aircraft for O_3 are compared with the simulated results.

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APPLICATION OF A THREE-DIMENSIONAL PHOTOCHEMICAL SMOG FORMATION MODEL TO THE TOKYO METROPOLITAN AREA

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INTRODUCTION

High O_3 concentrations are frequently observed in the Tokyo Metropolitan Area (TMA) in the summer season. The industrial complexes located in the Tokyo Bay area are the largest in Japan and are the major fixed sources of pollutants (NO, NO_2, SO_2, hydrocarbons, aerosols, etc.), while the Tokyo Metropolis is the largest contributor of pollutants from mobile sources. Almost 25% of the total NO_x emissions from all of Japan come from this area. In addition, the topography of the area is very complicated which leads to complex wind patterns. Reflecting these circumstances the relationships between the precursor emissions and the field-observed O_3 patterns are not clearly understood. Investigating these relationships requires the use of a three-dimensional photochemical air pollution simulation model.

Relatively high O_3 concentrations were observed during an episode on July 16 and 17, 1981 in the TMA. The stagnant meteorological conditions which existed then were mainly caused by the local sea and land wind circulation systems. To better understand the physical and chemical relationships at work during this particular episode the SAI-UAM was applied. This model has been used extensively in other applications of urban airshed modeling for photochemical smog.[1] Vertical cross-sections of simulated pollutant patterns are analyzed for the TMA domain, including the diurnal variation in the patterns. The effects of vertical meteorological conditions and the previous day's secondary pollutants are emphasized. Limited field-observed data from aircraft for O_3 are compared with the simulated results.

SIMULATION

The location and topography of the TMA are shown in Figure 1. The area modeled is shown in Figure 2. Each individual cell is 6.8 km wide and 5.5 km long. This is called six times standard mesh system which is based on the length of latitude, longitude of this area and widely used in Japan. The full horizontal domain is 27 by 30 cells with the outer ring of cells serving as boundary condition cells. There are five layers in the vertical; the depth of each layer is a function of the time of day. The bottom three layers simulated the mixing layer. However when the mixing layer exceeded 1 km in height the five layers

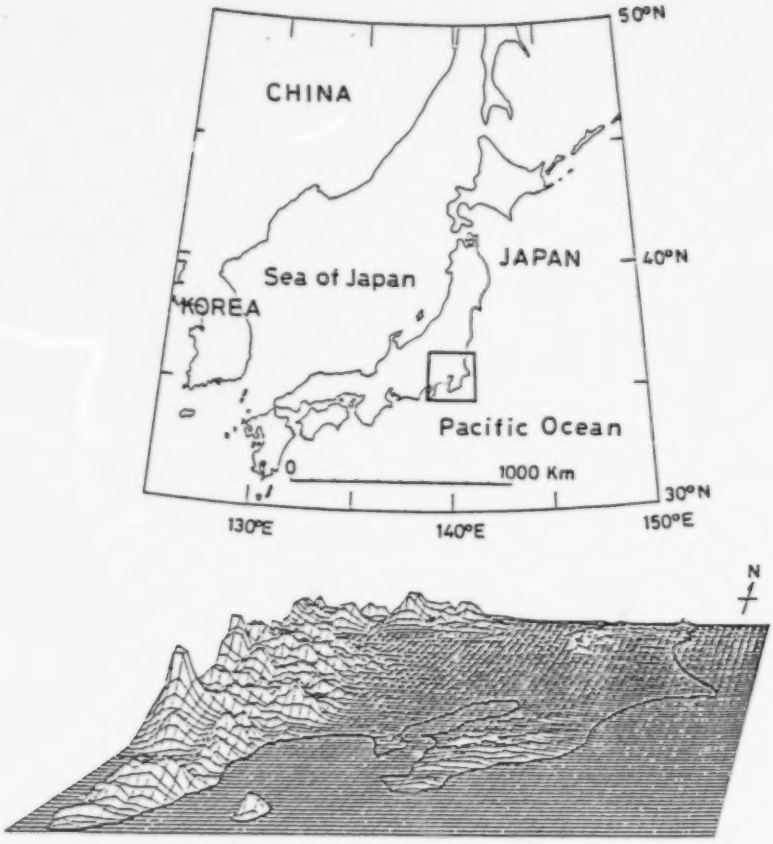

Figure1 Location of the Tokyo Metropolitan Area (TMA) and it's topography. Horizontalgrid size is 3 km square (not same size used in model simulation).

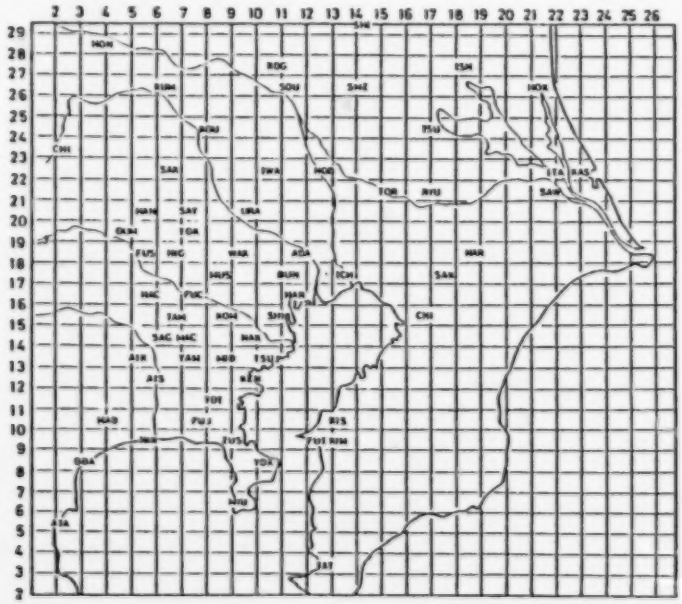

Figure 2 Schematic drawing of horizontal section of UAM domain. Acronyms in the figure show surface wind and airpollutants concentration monitoring stations.

were fixed at equal depths. The top height of the modeling domain was kept constant at 2 km. The basic equations of the UAM are:

$$\frac{\partial}{\partial t}(\Delta H c_i) + \frac{\partial}{\partial x}(u \Delta H c_i) + \frac{\partial}{\partial y}(v \Delta H c_i) + \frac{\partial}{\partial \rho}(W c_i)$$

$$= \frac{\partial}{\partial x}\left(K_H \Delta H \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \Delta H \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial \rho}\left(\frac{K_V}{\Delta H}\frac{\partial c_i}{\partial \rho}\right) + R_i \Delta H + S_i \Delta H$$

where

$$W = w - u\left(\frac{\partial h}{\partial x} + \rho \frac{\partial \Delta H}{\partial x}\right) - v\left(\frac{\partial h}{\partial y} + \rho \frac{\partial \Delta H}{\partial y}\right) - \rho \frac{\partial \Delta H}{\partial t}$$

$$\rho = \frac{z - h(x,y)}{\Delta H}$$

c_i = concentration of species i
ΔH = vertical increment in the modeling region
u,v,w = wind components in the x, y, and z directions, respectively
K_H, K_V = horizontal and vertical diffusivities
R_i = reaction rate term for species i
S_i = volumetric source term for species i
h(x,y) = terrain elevation.

Three-dimensional meteorological information (u, v, w, K_H, K_V) and source emissions data (S) must be prepared for the model in order to solve this equation. As shown in Figure 1, the western and northern sides of the TMA are walled by mountains 1-2 km high, while the other sides are open to the sea. Under a weak atmospheric pressure gradient, three different sea breeze regimes exist in separate parts of the area and create the extremely complicated wind patterns over the TMA. These local wind systems are the main influences on the patterns of vertical and horizontal pollutant distributions. In this study, the three-dimensional wind structure was estimated by data from 23 pilot balloon stations that had releases for 40 successive hours and a dense network of surface monitoring stations. The surface stations and pilot balloon sites are shown in Figures 2 and 3, respectively. To simulate the wind field three-dimensional mass and momentum-conserving wind model was used.[2] Another important meteorological parameter is the diurnal variation of mixing layer height. At the four upper-air sounding sites vertical temperature profiles were measured every two hours. Observed data at three of the four stations were averaged to determine the mixing height (see, for example, Figure 4).

The Carbon Bond II chemical kinetic scheme was used for the chemistry calculations in the UAM. Hourly emission rates were calculated from area sources and point sources for NO_x and non-methane hydrocarbons (NMHC) at each grid cell. The NMHC emissions must be distributed into particular reactivity classes. To accomplish this the ratio of 18 NMHC species from the five major hydrocarbon source categories (vehicle exhaust, oil refinery facilities, other petrochemical operations, gasoline vapor, and painting solvents) were determined.[3,4] Two large industrial complexes, Keihin and Keiyo, are located along Tokyo Bay, while the center of Tokyo is the largest contributor of pollutants from mobile sources. Model simulation was conducted for 40 hours beginning 0400JST, July 16, 1981. Initial and boundary pollutant concentrations are determined based on surface monitoring data and aircraft observation.

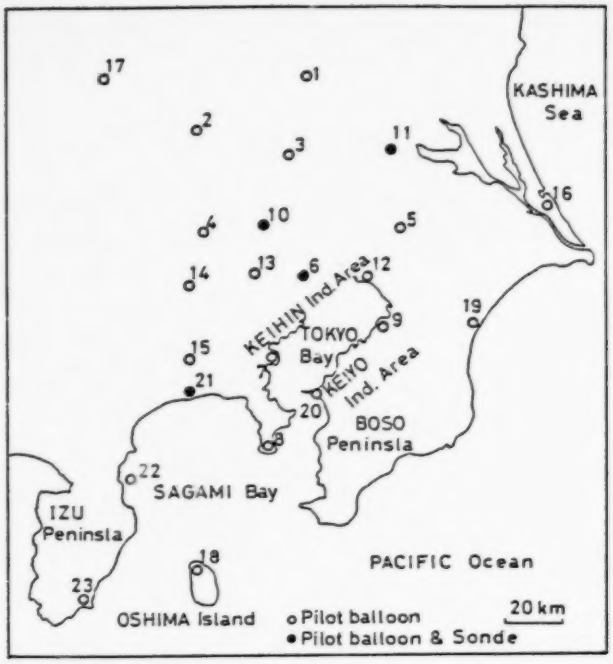

Figure 3 Upper wind and temperature monitoring stations.
Numerals in the figure show the following locations;
1) Oyama, 2) Kumagaya, 3) Satte, 4) Iruma, 5) Inzai,
6) Ootemachi, 7) Yokohama, 8) Miura, 9) Ichihara,
10) Urawa, 11) Tsukuba, 12) Tsudanuma, 13) Musashino,
14) Hachiouji, 15) Atsugi, 16) Kashima, 17) Takasaki,
18) Ooshima, 19) Kujukurihama, 20) Futtu, 21) Hiratsuka,
22) Hatsushima, 23) Shimoda.

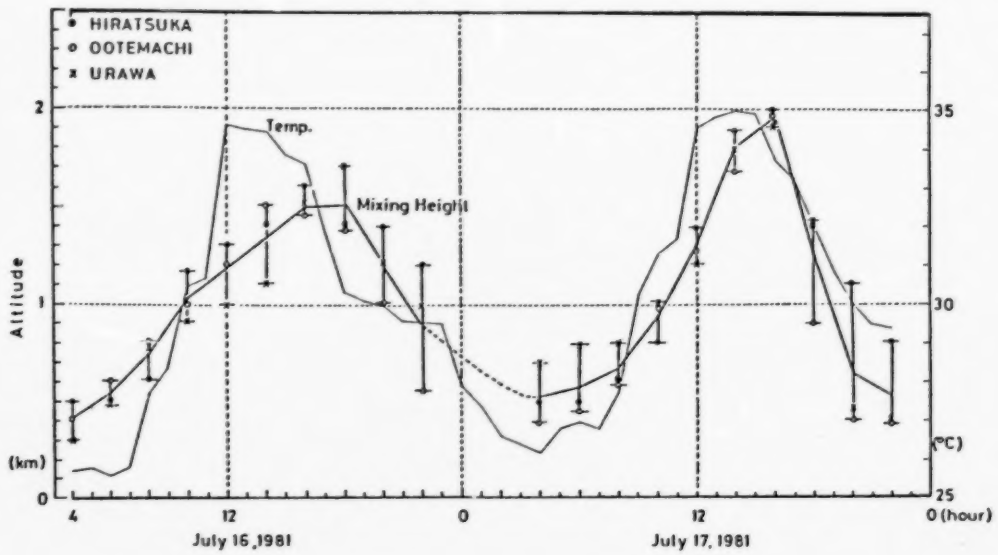

Figure 4 Diurnal variation of mixing height and surface temperature observed at Ootemachi.

RESULTS AND DISCUSSION

The predicted diurnal variation of O_3 and NO_2 concentrations for the two-day period along the North-South cross-section at the 9th mesh line from the western edge of the model domain (see Figure 2) is shown in Figure 5. This selected mesh line is corresponding to the aircraft flight course which is shown in Figure 8. At 1000JST on July 16, 1981, high NO_2 concentrations are predicted along the coastal area of Tokyo Bay reflecting the emissions from the Keihin Industrial Complex. Predicted O_3 concentrations, however, were especially low in this region of high NO_2 concentrations. At 1600JST predicted O_3 concentrations increased to 160 ppb and a sharp concentration gradient was observed at 1500 m. This altitude corresponds to the mixing height at the time, shown in Figure 4. The NO_2 concentration level was less than 10 ppb due to photochemical reaction and diffusion. After dark the NO_2 increased again near the surface in this area, while the O_3 concentrations were diminished by the quenching effects of the primary pollutants. At upper levels above the center of the model domain relatively high O_3 concentrations (140 ppb) remained on the evening of July 16. This polluted air mass was then transported to the southwestern portion of the model domain by 0400JST on July 17. At 1000JST on July 17 O_3 levels of over 100 ppb were calculated between the 4th and 9th North-South mesh lines. These concentrations here were quite different than those calculated for the previous day. The NO_2 levels were approximately the same here as on July 16. On July 17 the afternoon O_3 levels increased over those from the previous day and mixed well vertically through the higher mixing height of 2 km. After dark the same type of vertical O_3 patterns were observed with higher concentrations aloft.

Similar phenomena were also observed during the field study covering the TMA and the simulated results discussed here are consistent with the observations. Generally speaking, when the geostrophic wind at the 700 mb level is below 6 m/s, the local wind circulation system predominates and higher O_3 concentrations are observed at the southern part of the TMA.[5,6] On July 16 and 17, 1981 an easterly wind from the Kashima Sea and a southerly wind from Sagami Bay predominated in the daytime. There was a confluence of the southerly Sagami Bay breeze and the easterly wind from the Kashima sea. Under these conditions the primary pollutants from the Tokyo Bay coastal area and the Tokyo Metropolis were trapped in the southern part of the Kanto district. Aircraft data showing O_3 concentrations in excess of 200 ppb were observed near the coastal side of Sagami Bay between 1450-1455JST on July 16.

These characteristic features are well simulated by the UAM. According to this simulation the O_3 concentrations on the second day of the episode were higher than those on the first day. To aid in evaluating this prediction the diurnal variation of vertical profiles of NO_2, O_3, PAR (paraffins), and CARB (carbonyls) at Miura are shown in Figure 6. Miura is located mesh number (9,7) in the southern part of the domain. High NO_2 values are observed through the night with the maximum concentration at 300 m altitude on both nights. To investigate the hydrocarbons, the species PAR and CARB were selected. PAR and NO_2 show a close relative relationship with the highest values observed in the morning. On the other hand the maximum CARB concentrations are predicted aloft at night. In this simulation hydrocarbon emissions are only emitted at the surface; no elevated sources are considered. Therefore in the first day's simulation PAR and CARB concentrations show a maximum near the surface. However for the second day the maximum values are seen aloft from 300 m to 600 m, probably from the previous day's

carry-over effects. The largest difference between the two days is shown in the profiles of O_3 and CARB. In the second day especially high levels of these pollutants are observed during the night to early morning at altitudes between 300 and 600 m. These aged pollutants are entrained into the mixing layer in accordance with the elevation of the lid. Much higher O_3 concentrations are then produced as a result. Because of the higher CARB concentrations on the second day, the O_3 levels increased at an earlier time than on the first day.

Field observations of O_3 vertical profiles measured by aircraft are shown in Figure 7. The observations were performed between 1400JST and 1500JST on July 16, 1981. Ambient temperatures were measured at Ootemachi, and the locations where the vertical profiles were obtained are mapped in Figure 8. The aircraft observations show a sharp O_3 peak below the inversion layer especially at points A and B which are located near the sea. Near the coastal zone of Tokyo Bay there are numerous elevated NO_x emission sources such as power plants, oil refineries, petrochemical and steel industrial plants, etc. with stacks of height between 100 and 200 m. We will consider that NO_x from these emissions is trapped beneath the inversion layer and high O_3 concentrations are produced there. The simulated vertical O_3 distribution and observations at Miura (nearest station to point B) are shown in Figure 9. The simulated profile could not produce a sharp peak because of the coarse vertical resolution, but its qualitative characteristics are consistent with the observations.

CONCLUSIONS

To investigate the photochemical smog formation mechanism under stagnant meteorological conditions covering the TMA, the SAI-UAM was used to conduct air quality simulation for two such days. In a related study the SAI-UAM had produced reasonable areal and diurnal variations of O_3,[7,8] while in this study vertical distributions were mainly analyzed. Major efforts were devoted to clarify the effects of vertical meteorological conditions and the previous day's secondary pollutants on the second day's O_3 concentrations. Simulated results showed reasonable performance at reproducing a three-dimensional profile of O_3 concentrations.

In the TMA higher O_3 concentrations are usually observed near the shore in the morning. As the sea breeze layer penetrates inland, this high concentration region travels with it, increasing in concentration with time. The maximum O_3 concentrations are usually observed below the inversion layer. A nighttime radiation inversion that persists into the early morning prevents the dispersion of primary pollutants emitted from the large coastal industrial zones and the TMA. Usually, high O_3 concentration areas which are transported from inland by the nighttime land breeze are observed aloft in the early morning. These observational results were qualitatively reproduced by the UAM.

The role and significance of the previous day's secondary pollutants on O_3 formation mechanisms were investigated using UAM simulations. The largest differences in the vertical pollutant profiles between the two days studied were in the species O_3 and CARB. During the second night of simulation especially high values of these species were predicted above the radiation inversion layer. These aged pollutants were then entrained into the mixing layer during the day in accordance with the elevation of the lid. In part, because of the higher CARB concentration levels on the second day, O_3 levels increased earlier in time and peaked at higher concentrations than they had on the first day of simulation. The importance of the effects of the previous day's aged

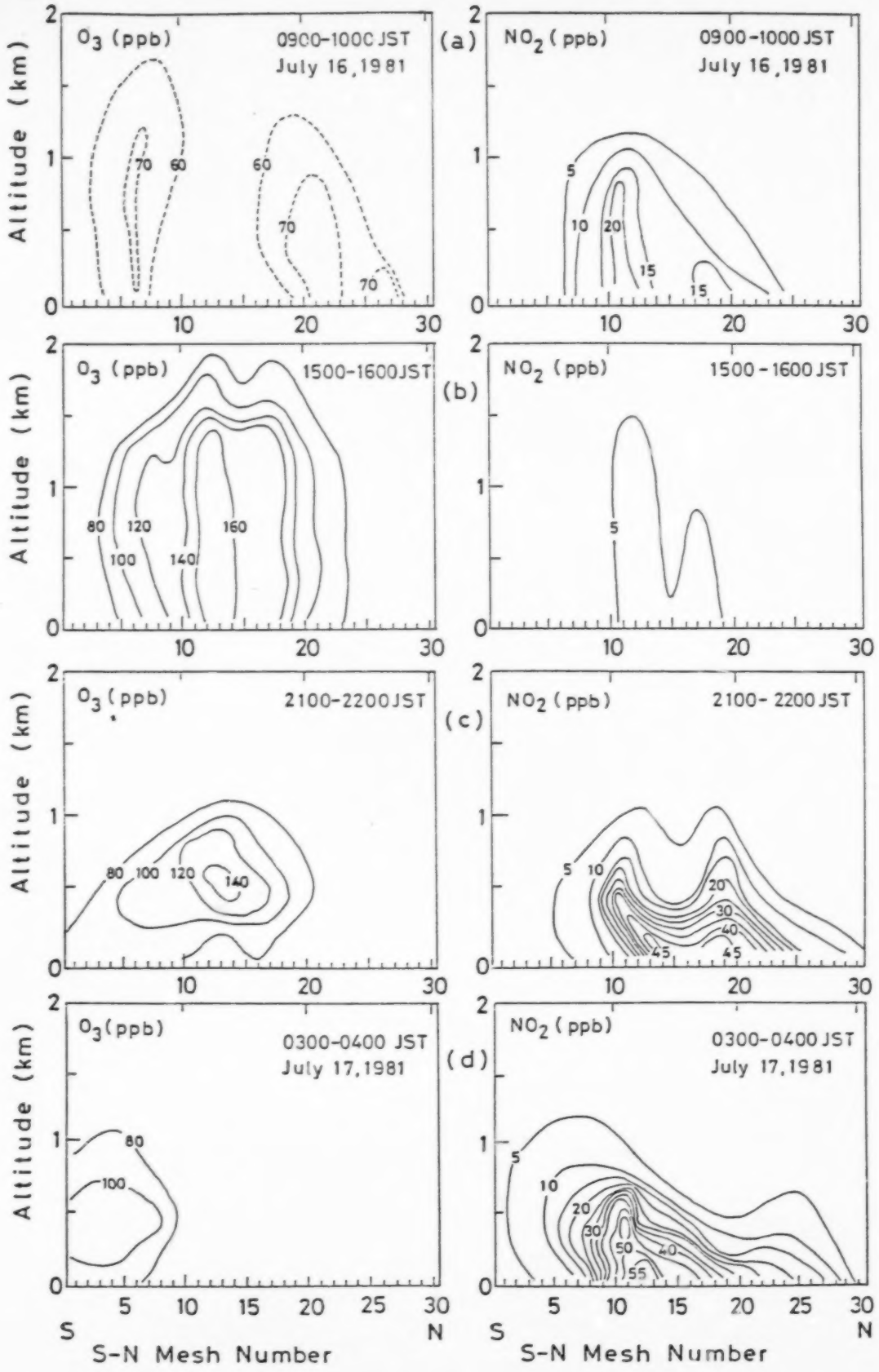
O3 (ppb)
0900-1000 JST
July 16, 1981
(a)
NO2 (ppb)
0900-1000 JST
July 16, 1981
O3 (ppb)
1500-1600JST
(b)
NO2 (ppb)
1500-1600 JST
O3 (ppb)
2100-2200JST
(c)
NO2 (ppb)
2100-2200 JST
O3 (ppb)
0300-0400 JST
July 17, 1981
(d)
NO2 (ppb)
0300-0400 JST
July 17, 1981
Altitude (km)
S-N Mesh Number
S
N

Figure 5

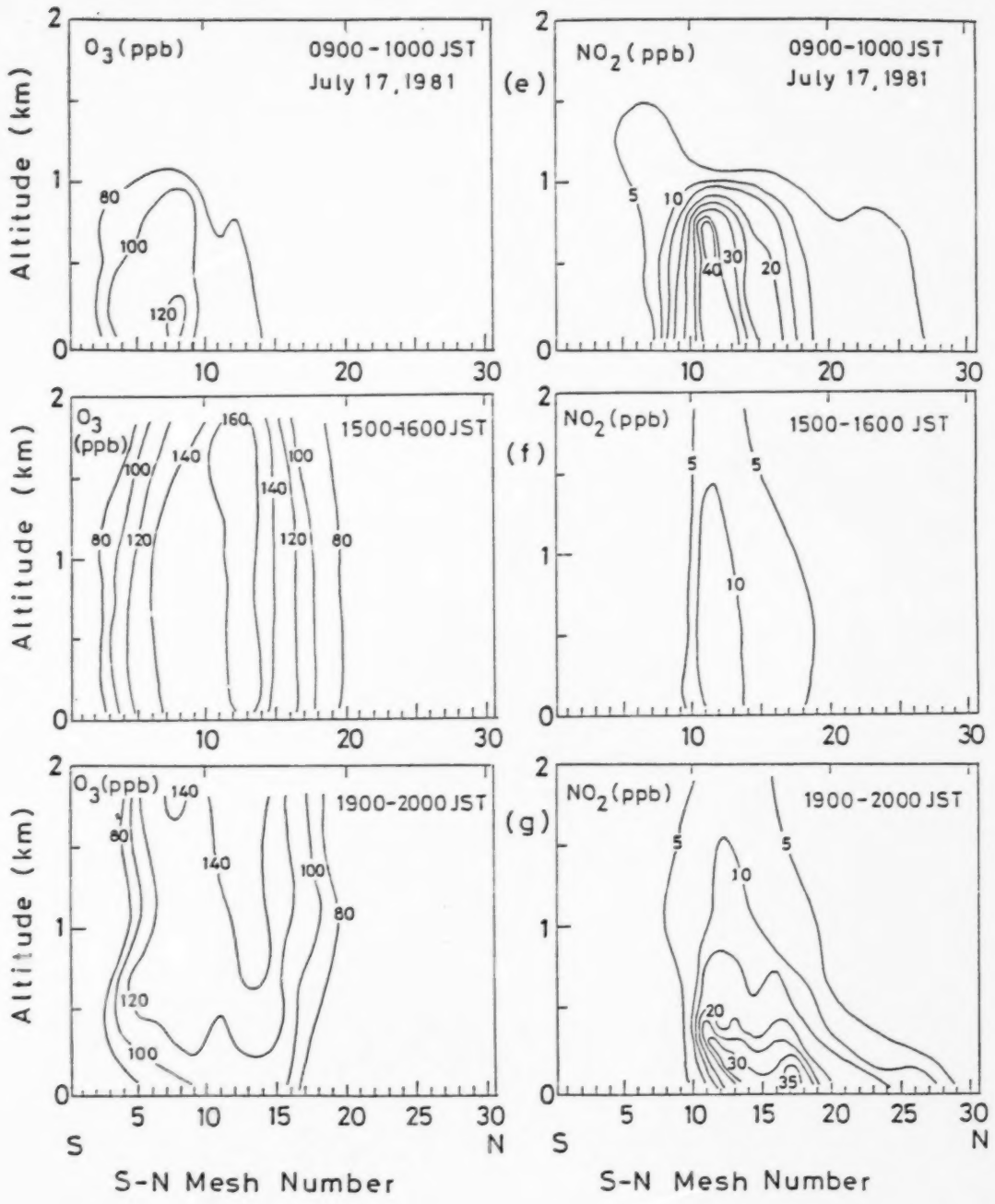

Figure 5 Vertical distribution of calculated O_3 and NO_2 concentrations along the S-N line of W-E mesh number 9.

a) 0900-1000JST July 16, 1981
b) 1500-1600JST July 16, 1981
c) 2100-2200JST July 16, 1981
d) 0300-0400JST July 17, 1981
e) 0900-1000JST July 17, 1981
f) 1500-1600JST July 17, 1981
g) 1900-2000JST July 17, 1981

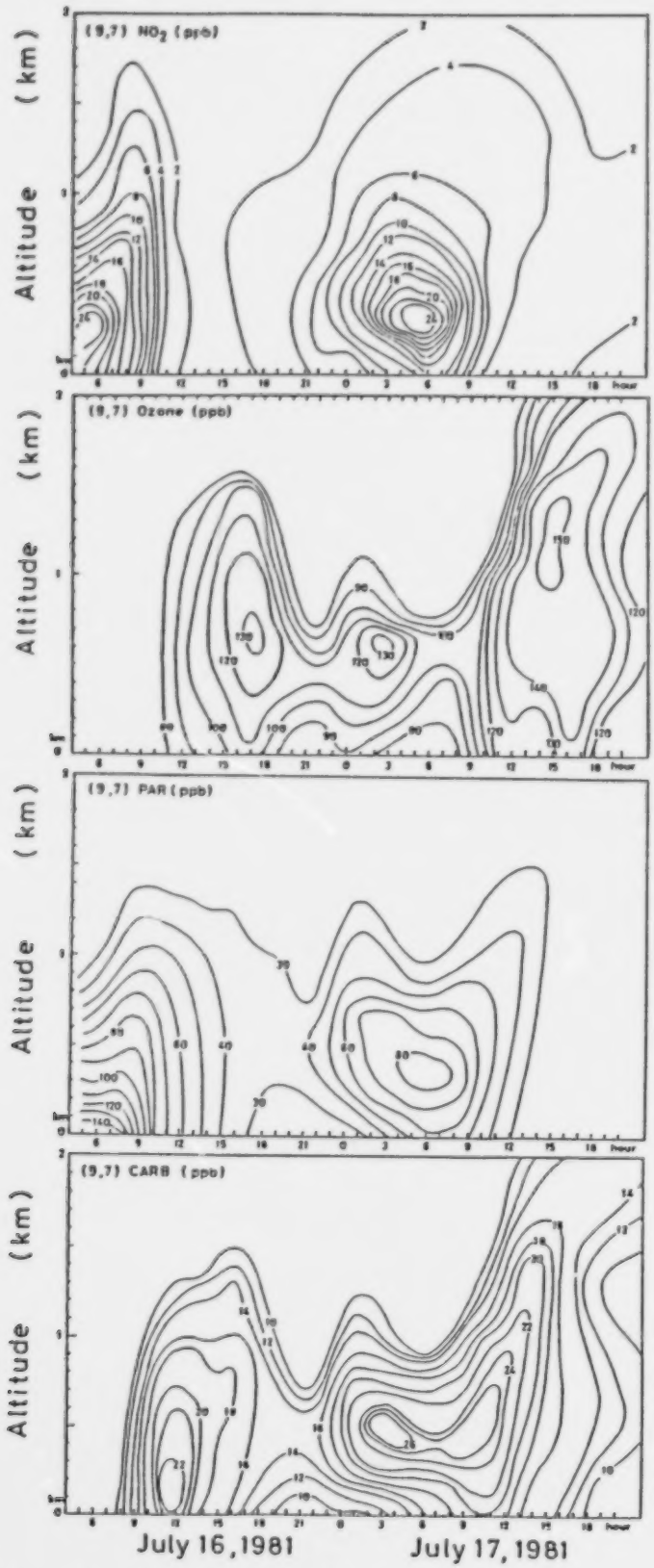

Figure 6 Diurnal variation of vertical profiles of NO_2, O_3, PAR (Paraffin) and CARB (Carbonyl compounds) concentrations at Miura. Miura is located at the mesh point (9,7).

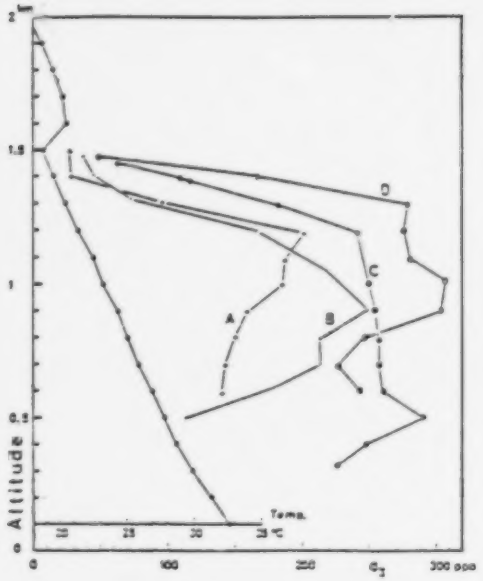

Figure 7 Vertical distribution of O_3 measured by aircraft on July 16, 1981 around the Tokyo Bay area, and temperature profile at Ootemachi, 1420JST.

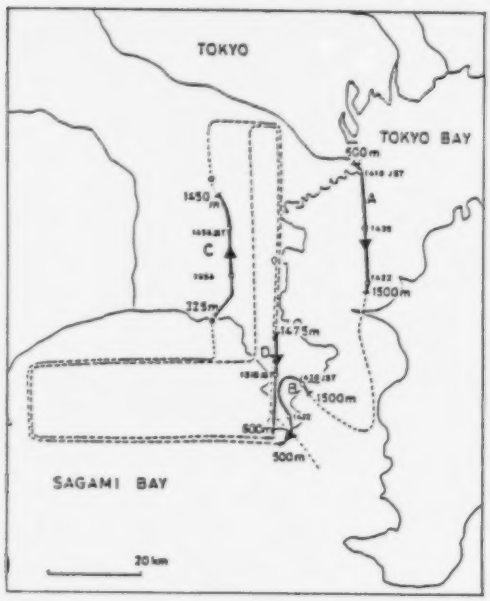

Figure 8 Aircraft flight course on July 16, 1981. Numerals in the figure show altitude and time in JST.

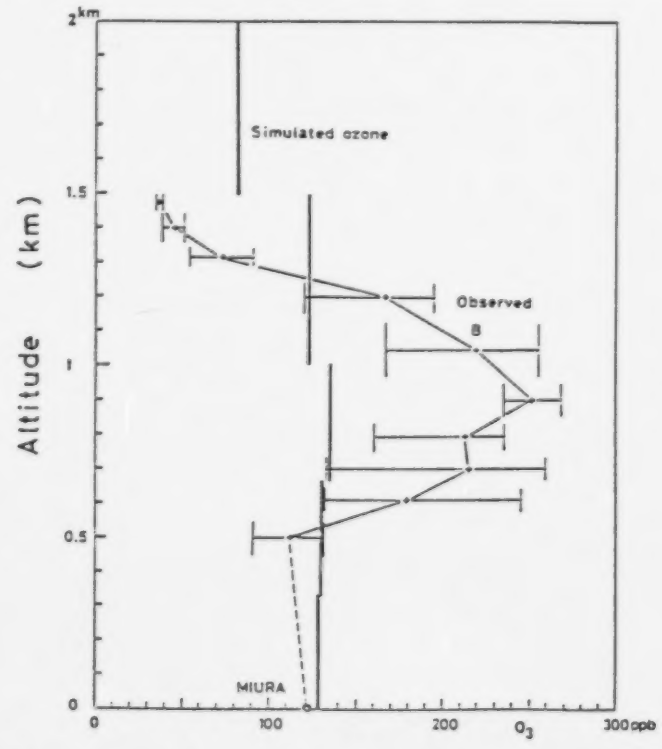

Figure 9 Comparison between the simulated vertical O_3 distribution and observations at Miura. Miura is the nearest surface monitoring station to aircraft sampling point B which is shown in Figure 8.

pollutants are confirmed using the UAM. Observed vertical O_3 profiles were also compared with the simulation results. The simulated vertical profiles were in qualitative agreement with the observations although the coarse vertical resolution and hour averaging in the model may have prevented the prediction of the maximum concentrations accurately.

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